Waves in Open Systems via Bi-orthogonal Basis

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(February 7, 2008)

Dissipative quantum systems are sometimes phenomenologically described in terms of a non-hermitian hamiltonian H, with different left and right eigenvectors forming a bi-orthogonal basis. It is shown that the dynamics of waves in open systems can be cast exactly into this form, thus providing a well-founded realization of the phenomenological description and at the same time placing these open systems into a well-known framework. The formalism leads to a generalization of norms and inner products for open systems, which in contrast to earlier works is finite without the need for regularization. The inner product allows transcription of much of the formalism for conservative systems, including perturbation theory and second-quantization.

PACS numbers: 03.40.Kf, 02.30.Mv, 02.60.Lj, 03.65.-w

Introduction

Dissipative systems can be discussed in many ways. The fundamental approach recognizes that energy flows from the system S to a bath B, whose degrees of freedom are then eliminated from the path integral or equations of motion [1]. While rigorous, this approach is inevitably complicated, and often leads to integro-differential equations for time evolution. An alternate phenomenological approach *postulates* a non-hermitian hamiltonian (NHH) H, whose left and right eigenvectors form a bi-orthogonal basis (BB) [2–7]. These NHHs with discrete BBs can sometimes be obtained from a full quantum theory, but usually under some approximations [5,8].

This Letter discusses a class of models of waves in open systems. These are scalar fields $\phi(x,t)$ in 1 d, described by the wave equation. Outgoing wave boundary conditions cause the system to be dissipative. We show that these open systems are *exactly* described by an NHH with a BB formed by the resonances or quasinormal modes (QNMs). This connection on the one hand provides the phenomenological approach with a realization which has an impeccable pedigree rigorously traceable to the fundamental approach, and on the other hand places earlier work on such open systems into a familiar framework. A generalized inner product emerges; in contrast to previous works, it is finite and requires no regularization. Under the generalized inner product, the hamiltonian H is symmetric, which opens the way to a clean formulation of perturbation theory and second-quantization in terms of the QNMs of the system.

Waves in Open Systems

We consider waves in 1 d described by $\left[\rho(x)\partial_t^2 - \partial_x^2\right]\phi(x,t) = 0$ on the half line $[0,\infty)$, with $\phi(x=0,t) = 0$ and $\phi(x,t)$ approaching zero rapidly as $x \to \infty$ [9]. Let the system S be the "cavity" $I = [0,a]$, and the bath B be (a,∞), where $\rho(x) = 1$. Energy is exchanged between S and B only through the boundary $x = a$. We impose the outgoing wave condition $\partial_t\phi(x,t) = -\partial_x\phi(x,t)$ for $x > a$.

This mathematical model is relevant for many physical systems: the vibrations of a string with mass density ρ [10]; the scalar model of EM in an optical cavity (the node at $x = 0$ is a totally reflecting mirror, and a partially transmitting mirror at $x = a$ can be modeled by $\rho(x) = M\delta(x-a)$) [11]; or gravitational radiation from a star with radius a [12]. The wave equation can be mapped to the Klein-Gordon equation with a potential $V(x)$ [13], which is relevant for gravitational waves [14]; here ϕ is the perturbation about the spherical background metric of a star, x is a radial coordinate related to the circumferential radius r, and V describes the wave scattering by the background metric. Gravitational waves carrying the signature of the QNMs of black holes may soon be observed by new detectors such as LIGO and VIRGO [15].

For the "cavity" $I = [0,a]$, the outgoing condition is imposed at $x = a^+$ only. The QNMs are factorized solutions on I: $\phi(x,t) = f_n(x)e^{-i\omega_n t}$, with $[\partial_x^2 + \rho(x)\omega_n^2]\, f_n(x) = 0$. These are observed in the frequency domain as resonances of finite width (e.g., the EM spectrum seen outside an optical cavity) or in the time domain as damped oscillations (e.g., the numerically simulated gravitational wave signal from the vicinity of a black hole). It would obviously be interesting to be able to describe these QNMs in a manner parallel to the normal modes (NM) of a conservative system.

These QNMs form a complete set on I if (a) $\rho(x)$ has a discontinuity at $x = a$ to provide a natural demarcation of the "cavity", and (b) $\rho(x) = 1$ for $x > a$, so that outgoing waves are not scattered back into the system [16]. Under these conditions, one can expand $\phi(x,t) = \sum_n a_n f_n(x)e^{-i\omega_n t}$ for $x \in I$ and $t \geq 0$, thus

allowing an *exact* description of the system in terms of *discrete* variables (modes spaced by $\Delta\omega \sim \pi/a$) rather than a continuum. Nevertheless, the analogy with conservative systems is still not apparent: Is there a natural inner product (with which to do projections and thus to prove the uniqueness of expansions)? Is there a norm to scale wavefunctions (noting that f_n diverges at spatial infinity)? Can perturbation theory be formulated (noting that the usual proofs require an inner product to define orthogonality)? Can the theory be second-quantized? This Letter shows that all these questions have natural answers in the language of a BB.

Phenomenological non-Hermitian Hamiltonians and Bi-orthogonal Bases

Though not rigorously founded upon a genuine quantum theory, NHHs with BBs are nevertheless well developed as a *postulatory* system [2,3]. Consider a space W on which is defined a non-hermitian operator H and a conjugate linear duality transformation D: $D\left(\alpha|\Phi\rangle + \beta|\Psi\rangle\right) = \alpha^* D\,|\Phi\rangle + \beta^* D\,|\Psi\rangle$, such that $DH = H^\dagger D$ [17]. The BB consists of the two set of eigenvectors $|F_n\rangle \in W$ and $|G_n\rangle = D\,|F_n\rangle \in \tilde{W} = D(W)$ satisfying $H\,|F_n\rangle = \omega_n\,|F_n\rangle$, $H^\dagger\,|G_n\rangle = \omega_n^*\,|G_n\rangle$, where the two eigenvalues are related by duality. By projecting the eigenvalue equations on $\langle G_n|$ and $|F_n\rangle$, it follows easily that $\langle G_n|F_m\rangle = 0$, for $m \neq n$.

It is usually assumed that these eigenstates are complete, so that any vector can be expanded as $|\Phi\rangle = \sum_n a_n\,|F_n\rangle$, with $a_n = \langle G_n|\Phi\rangle/\langle G_n|F_n\rangle$, leading immediately to the resolution of the identity and of the time-evolution operator

$$1 = \sum_n \frac{|F_n\rangle\langle G_n|}{\langle G_n|F_n\rangle} \tag{1}$$

$$e^{-iHt} = \sum_n \frac{|F_n\rangle e^{-i\omega_n t}\langle G_n|}{\langle G_n|F_n\rangle} \tag{2}$$

which in principle solves all the dynamics [18].

Bi-orthogonal Basis for the Wave Equation

BBs are widely used in many disciplines, for example in the theory of wavelets [19] and to describe excited molecular systems [4,20]. The left and right eigenvectors of the Maxwell operator are typically used to represent the Green's function for EM fields in open cavities [21–23], or to evaluate Fox-Li states [24]. Here we seek a parallel with quantum mechanics, similar to earlier works for generalized oscillators [25] and the classical wave equation (without dissipation due to leakage) [26]. The problem at hand, where there is dissipation due to outgoing waves, was formulated in this manner recently [27], and is briefly sketched below, especially as it relates to the BB.

It is natural to introduce the conjugate momentum $\hat{\phi} = \rho(x)\partial_t\phi$, and the two-component vector $|\Phi\rangle = (\phi, \hat{\phi})^{\mathrm{T}}$. In terms of this, the dynamics can be cast into the Schrödinger equation with the NHH

$$H = i\begin{pmatrix} 0 & \rho(x)^{-1} \\ \partial_x^2 & 0 \end{pmatrix} \tag{3}$$

The identification $\hat{\phi} = \rho\partial_t\phi$ follows from the evolution equation [28].

The natural definition of an inner product between $|\Psi\rangle = (\psi, \hat{\psi})^{\mathrm{T}}$ and $|\Phi\rangle = (\phi, \hat{\phi})^{\mathrm{T}}$ on $[0, \infty)$ is

$$\langle\Psi|\Phi\rangle = \int_0^\infty \left(\psi^*\phi + \hat{\psi}^*\hat{\phi}\right) dx \tag{4}$$

However, on account of the assumed asymptotic behavior, the integral is convergent.

For outgoing waves, we consider only the space U of such vectors $|\Phi\rangle$ defined on $[0, \infty)$ which satisfy the outgoing condition $\hat{\phi} = -\phi'$ for $x > a$. The bath variables are eliminated simply but exactly by projecting to the space W of vectors $|\Phi\rangle$ defined on I and which satisfy $\hat{\phi} = -\phi'$ at $x = a^+$. The QNMs are right-eigenvectors of H: $|F_n\rangle \equiv (f_n, \hat{f}_n)^{\mathrm{T}} = (f_n, -i\omega_n\rho f_n)^{\mathrm{T}}$. The duality transformation is $D\,(\phi_1, \phi_2)^{\mathrm{T}} = -i(\phi_2^*, \phi_1^*)^{\mathrm{T}}$.

For open systems, a crucial concept is the inner product between one vector and the dual of another, to which we give a compact notation:

$$(\Psi, \Phi) \equiv \langle D\Psi|\Phi\rangle = i\int_0^\infty \left(\hat{\psi}\phi + \psi\hat{\phi}\right) dx \tag{5}$$

which is linear in both vectors, and cross-multiplies the two components, properties to be emphasized below. This bilinear map plays the role of the inner product for conservative systems.

Our notation does not distinguish between functions (say $|\Phi\rangle$) defined on $[0, \infty)$ and their restrictions to I; the former are in U and the latter are in W, with the association between them being many-to-one. As written in (5), the inner product involves the wavefunctions outside I, i.e., it appears to be defined on U rather than W. However, one can completely eliminate the bath degrees of freedom: because of the outgoing conditions, the integrand on (a, ∞) reduces to a total derivative, and (5) can be written purely in terms of the inside variables [27]:

$$(\Psi, \Phi) = i\left\{\int_0^{a^+} \left(\hat{\psi}\phi + \psi\hat{\phi}\right) dx \;+\; \psi(a^+)\phi(a^+)\right\} \tag{6}$$

The surface term is the only remnant of the outside. Thus, (6) can be regarded as a bilinear map (or loosely an inner product) defined on W [27]. The somewhat peculiar structure (e.g., the cross-multiplication between the two components and the appearance of the surface term) is now seen to arise naturally from (4) upon the introduction of the duality transformation. In the limit where the escape of the waves is small, the generalized norm of an eigenvector (F_n, F_n) reduces to $2\omega_n$ times the conventional norm; this is the reason for choosing the

phase convention for D. The ability to normalize QNM wavefunctions is nontrivial, since f_n diverges at spatial infinity, and a naive expression such as $\int_0^\infty |f_n|^2 dx$ would not be appropriate.

The diagonal version (Φ, Φ) for the special case of QNMs was first introduced by Zeldovich [29] in a form that involved (a) ϕ outside I (so that it is defined on U rather than W) and (b) regularization of the divergent integral rather than a surface term; it was later re-cast into the form (6) and generalized to 3 d and EM fields [30]. The off-diagonal form (Ψ, Φ) was later introduced [27]. Here, by relating the discussion to bi-orthogonal states and the duality transformation, it is seen that these concepts emerge naturally, including the specific form of (6).

An inner product equivalent to (6) has also been discussed extensively from other perspectives [31,32]. In these works, the inner product is defined on $[0, \infty)$ rather than a finite interval, with the consequent divergence (e.g., for the inner product between two QNMs each growing exponentially at infinity) handled either (a) by a regulating factor $\exp(-\epsilon x^2)$, $\epsilon \to 0^+$, (b) analytic continuation in the wavenumber k, or (c) complex rotation in the coordinate x. Each of these procedures has its limitations; in contrast, (6) makes no reference to the outside or bath, and is computationally convenient and manifestly finite.

Under this bilinear map, H is symmetric: $(\Psi, H\Phi) = (\Phi, H\Psi)$, which follows very simply from $DH = H^\dagger D$. This key property is analogous to the hermiticity of H for conservative systems. It is nontrivial, in that surface terms that arise in the integration by parts are exactly compensated by the surface terms in (6). This symmetry property leads, in the usual way, to the orthogonality of non-degenerate eigenfunctions.

The completeness relation (1) is a dyadic equation. Its $(1,2)$ and $(1,1)$ components lead to the sum rules [34]

$$\sum_n \frac{f_n(x) f_n(y)}{2\omega_n} = 0$$

$$\sum_n \frac{1}{2} f_n(x) f_n(y) \rho(x) = i\delta(x-y) \tag{7}$$

for $x, y \in I$, which have been derived and discussed extensively [27].

The completeness and orthogonality relationships establish the QNMs as a BB, and moreover allow the time evolution to be solved as $|\Phi(x,t)\rangle = \sum_n a_n e^{-i\omega_n t} |F_n\rangle$, where $a_n = \langle G_n | \Phi(x,0)\rangle / (2\omega_n)$. This is a *discrete* and *exact* representation of the dynamics, even though I is open to an infinite universe with a continuum of states. Completeness is not proved in most other applications of NHHs to physical systems.

Perturbation theory

These notions allow much of the standard formalism in quantum mechanics to be carried over. As one example consider time-independent perturbation theory. Let $\rho_0(x)^{-1}$ be changed to $\rho(x)^{-1} = \rho_0(x)^{-1}[1 + \mu V(x)]$, where $|\mu| \ll 1$ $V(x)$ has support in I. Then the perturbation to the eigenvalues and eigenfunctions can be written in the standard Rayleigh-Schrödinger form, in terms of a *discrete* series [27]. These formulas, though superficially identical with textbook formulas for conservative systems, are nontrivial in two ways. First, the perturbative formulas apply to *complex* eigenvalues. Second, the use of resonances implies that there is no "background", and expressing the corrections in terms of discrete modes also means that the small parameter of expansion is $\mu/|\Delta\omega| \sim \mu a/\pi$, which would not have been apparent in terms of the states of the continuum.

The derivation of these results simply follows the conservative case (everywhere replacing inner products by the bilinear map (Ψ, Φ)), and need not be repeated.

Discussion

We have established an exact correspondence between phenomenological NHHs and waves in a class of open systems. This relationship provides a well-founded realization of NHHs. Because we start with a hamiltonian system and remove the bath degrees of freedom without approximations, these open systems can be second-quantized [35]. In other words, one can discuss photons in open cavities using BBs, which makes this class of examples unique and interesting. The relationship also places these open systems into a well-known and convenient framework. Thus, the linear space structure, orthogonality and completeness can all be derived naturally, by transcribing usual derivations for conservative systems and everywhere replacing the inner product by (Ψ, Φ).

The formalism discussed here also applies to the Klein-Gordon equation with a potential $V(x)$ [13], which applies, among other things, to linearized gravitational waves propagating away from a black hole. The first-order perturbation result for the QNM frequencies has been used to understand the shifts in the gravitational wave frequencies when a black hole is surrounded by an accretion shell [33].

The wave equation discussed here may be regarded as a physical realization of BBs for open systems. Many other inequivalent realizations arise when one considers outgoing waves in a spherically symmetric 3-d system; each angular momentum l leads to realizations in which the surface terms in the inner product involves l radial derivatives [36].

However, the entire formalism refers to systems described by second-order differential equations, so that two sets of initial data, namely ϕ and $\hat{\phi}$, are required, and the outgoing condition is expressed as a constraint between them. The formalism does *not* apply in its entirety to systems described by first-order differential equations, e.g., α-decays described by the Schrödinger equation with Gamow boundary condition. In any event,

the Schrödinger equation formally gives unbounded signal speeds and does not possess outgoing and incoming sectors related by time reversal; thus the concept of outgoing waves is actually quite different. Nevertheless, if one is interested only in frequency domain problems, e.g., eigenvalue problems and time-independent perturbation theory, then the formalism survives even in this case. This is most easily appreciated by starting with the Klein-Gordon equation and simply relabelling $\omega^2 \mapsto \omega$.

Using (Ψ, Φ) rather than the equivalent form $\langle D\Psi|\Phi\rangle$ allows all reference to D to be avoided. However, (Ψ, Φ) is a bilinear map (rather than being linear in the ket and conjugate linear in the bra). This property is quite general, since D is conjugate linear. But in most applications of the inner product (e.g., for projections), it does not matter whether the map is linear or conjugate linear in the bra; this is why results from conservative systems can be carried over. The only property that is lost is the positivity of (Φ, Φ), which is unsurprising for a dissipative system. Thus it is useful to think of the states of quantum dissipative systems as vectors in a linear space W endowed with such a bilinear map, which is the generalization of the notion of a Hilbert space. Time-evolution is then generated by an operator H which is symmetric.

The open systems described here are genuinely dissipative, with $\mathrm{Im}\,\omega_n < 0$. This contrasts with some models with NHHs which are nevertheless conservative [25,26]. For infinite-dimensional NHH models, completeness of the BB is usually *assumed*, but difficult to prove. Through these wave systems, we have provided explicit examples where completeness can be proved (if the discontinuity and "no tail" conditions are met), as well as examples where the basis is not complete (if these conditions are not met). These should also be useful in furthering understanding of NHH models.

We thank C. K. Au, E. S. C. Ching, S. Y. Liu and A. Maassen van den Brink for discussions. This work is supported in part by the Hong Kong Research Grants Council (Grant no. 452/95P). The work of WMS is also supported by the US NFS (Grant no. PHY 96-00507), and by the Institute of Mathematical Sciences of The Chinese University of Hong Kong. The work of CPS at The Chinese University of Hong Kong is also supported by a C. N. Yang Fellowship.

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